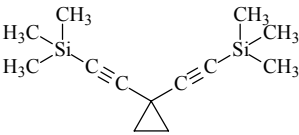


921 **C₁₃H₂₂Si₂**ED, vibrational spectroscopy,
ab initio calculations**(Cyclopropylidenedi-2,1-ethynediyl)bis-**
(trimethylsilane)

1,1-Bis(trimethylsilyl)ethynylcyclopropane

C_{2v} assumed (*syn*)

$r_{\text{hl}}^{\text{a)}$	$\text{\AA}^{\text{b)}$	$\theta_{\text{hl}}^{\text{a)}$	$\text{deg}^{\text{b)}$	
Si–C(m) ^{c)}	1.877(1) ^{d)}	C(2')–C(1)–C(2'')	117.1(7)	
Si–C(1')	1.835(3)	C(1')–Si–C(m)	108.3 ^{d)} ^{e)}	
C(1')≡C(2')	1.239(1)	Si–C–H	112.5(4)	
C(2')–C(1)	1.446(2)			
C(1)–C(2)	1.545(3)			
C(2)–C(3)	1.482(6)			
C(m)–H ^{c)}	1.105(1)			
C–H (ring) ^{c)}	1.095 ^{f)}			

An ED analysis based on a model of C₂ symmetry, with small deviations from the C_{2v} model (*syn*, *i.e.*, one C(m)–Si eclipsing C(1)–C(2')), gave identical results with those based on the C_{2v} model. The Si–C≡C–C fragments were assumed to be linear. According to RHF/6-311G** calculations, the torsion of the trimethylsilyl groups is virtually free. The nozzle temperature was 87...88 °C.

^{a)} Nonlinear kinematic effects were taken into account.

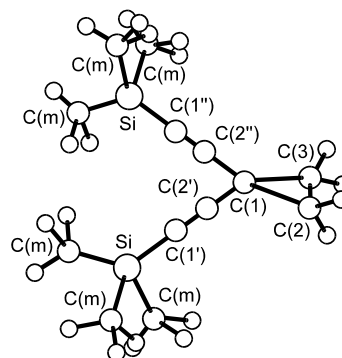
^{b)} Uncertainties were not specified, probably estimated standard errors.

^{c)} Average value.

^{d)} Differences in the Si–C(m) distances and in the C(1')–Si–C(m) bond angles were assumed at the values from MP2/6-311G** calculations.

^{e)} Assumed in the final refinement.

^{f)} Difference between the C(m)–H and C–H (ring) distances was assumed at the value from MP2/6-311G** calculations.



Trætterberg, M., Khaikin, L.S., Grikin, O.E., Kozhushkov, S.I., de Meijere, A.: J. Mol. Struct. **641** (2002) 41.

See also: de Meijere, A., Kozhushkov, S.I., Boese, R., Haumann, T., Yufit, D.S., Howard, J.A.K., Khaikin, L.S., Trætterberg, M.: Eur. J. Org. Chem. (2002) 485.